



ADIPIC ACID (3,3,4,4-D4, 98%)

Safety Data Sheet

according to Regulation (EC) No. 453/2010 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Date of issue: 25/01/2011

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Supersedes: 08/03/2012

Version: 3.0

DLM-2632

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

Product form : Substance
Substance name : ADIPIC ACID (3,3,4,4-D4, 98%)
EC index no : 607-144-00-9 (Unlabeled)
EC no : 204-673-3 (Unlabeled)
CAS No : 121311-78-2
Product code : DLM-2632
Formula : HOOCCH₂(CD₂)₂CH₂COOH
Synonyms : Hexanedioic acid

1.2. Relevant identified uses of the substance or mixture and uses advised against

1.2.1. Relevant identified uses

Main use category : Professional use
Industrial/Professional use spec : For professional use only.

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

Cambridge Isotope Laboratories, Inc.
50 Frontage Road
Andover, MA 01810
USA

USA: 1-800-322-1174 Int: 1-978-749-8000
cilsales@isotope.com www.isotope.com

Emergency telephone number

Emergency numbers:

Chemtrec: 1-800-424-9300 (24 hours)
International: 1-703-741-5970 (24 hours)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Eye Irrit. 2 H319

Full text of H-phrases: see section 16

Classification according to Directive 67/548/EEC or 1999/45/EC

Xi; R36
R52

Full text of R-phrases: see section 16

Classification (GHS-US)

Eye Irrit. 2A H319
Aquatic Acute 3 H402

Adverse physicochemical, human health and environmental effects

No additional information available

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2.2. Label elements

Labeling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :



GHS07

Signal word (CLP) : Warning

Hazard statements (CLP) : H319 - Causes serious eye irritation

Precautionary statements (CLP) : P264 - Wash Both hands thoroughly after handling
P280 - Wear protective clothing, protective gloves
P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P337+P313 - If eye irritation persists: Get medical advice/attention
P501 - Dispose of contents/container to Comply with applicable regulations.

GHS-US labeling

Hazard pictograms (GHS-US) :



GHS07

Signal word (GHS-US) : Warning

Hazard statements (GHS-US) : H319 - Causes serious eye irritation
H402 - Harmful to aquatic life

Precautionary statements (GHS-US) : P264 - Wash Both hands thoroughly after handling
P273 - Avoid release to the environment
P280 - Wear protective clothing, protective gloves
P305+P351+P338 - If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P337+P313 - If eye irritation persists: Get medical advice/attention
P501 - Dispose of contents/container to Comply with applicable regulations.

2.3. Other hazards

No additional information available

SECTION 3: Composition/information on ingredients

3.1. Substances

| Name | Product identifier | % | Classification according to Directive 67/548/EEC |
|---|---|-----|---|
| ADIPIC ACID (3,3,4,4-D4, 98%) (Main constituent) | (CAS No) 121311-78-2 (EC no) 204-673-3 (Unlabeled) (EC index no) 607-144-00-9 (Unlabeled) | 100 | Xi; R36 R52 |
| Name | Product identifier | % | Classification according to Regulation (EC) No. 1272/2008 [CLP] |
| ADIPIC ACID (3,3,4,4-D4, 98%) (Main constituent) | (CAS No) 121311-78-2 (EC no) 204-673-3 (Unlabeled) (EC index no) 607-144-00-9 (Unlabeled) | 100 | Eye Irrit. 2, H319 |

Full text of R-, H- and EUH-phrases: see section 16

| Name | Product identifier | % | Classification (GHS-US) |
|---|----------------------|-----|--|
| ADIPIC ACID (3,3,4,4-D4, 98%) (Main constituent) | (CAS No) 121311-78-2 | 100 | Eye Irrit. 2A, H319 Aquatic Acute 3, H402 |

Full text of H-phrases: see section 16

3.2. Mixtures

Not applicable

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SECTION 4: First aid measures

4.1. Description of first aid measures

- First-aid measures general : Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.
- First-aid measures after inhalation : If breathed in, move person to fresh air. If not breathing, give artificial respiration. Consult a physician.
- First-aid measures after skin contact : Wash off with soap and plenty of water. Consult a physician.
- First-aid measures after eye contact : Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.
- First-aid measures after ingestion : Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2. Most important symptoms and effects, both acute and delayed

- Symptoms/injuries after inhalation : May be harmful if inhaled. Causes respiratory tract irritation.
- Symptoms/injuries after skin contact : May be harmful if absorbed through skin. May cause skin irritation.
- Symptoms/injuries after eye contact : Causes eye irritation.
- Symptoms/injuries after ingestion : May be harmful if swallowed.

4.3. Indication of any immediate medical attention and special treatment needed

No additional information available

SECTION 5: Firefighting measures

5.1. Extinguishing media

- suitable extinguishing media : Use water spray, alcohol-resistant foam, dry chemical, or carbon dioxide.

5.2. Special hazards arising from the substance or mixture

- Fire hazard : Not available.

5.3. Advice for firefighters

- Firefighting instructions : Wear self contained breathing apparatus for fire fighting if necessary.
- Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

- Protective equipment : Ensure there is adequate ventilation.
- Emergency procedures : Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Avoid breathing dust.

6.1.2. For emergency responders

No additional information available

6.2. Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3. Methods and material for containment and cleaning up

- For containment : Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4. Reference to other sections

No additional information available

SECTION 7: Handling and storage

7.1. Precautions for safe handling

- Precautions for safe handling : Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs. Provide appropriate exhaust ventilation at places where dust is formed.
- Hygiene measures : Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

7.2. Conditions for safe storage, including any incompatibilities

- Technical measures : Keep container tightly closed in a cool, dry and well-ventilated place.
- Storage conditions : Store at room temperature away from light and moisture.

7.3. Specific end use(s)

No additional information available

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SECTION 8: Exposure controls/personal protection

8.1. Control parameters

ADIPIC ACID (3,3,4,4-D4, 98%) (121311-78-2)

| | | |
|------------------------------|--------------------------------------|---|
| Italy - Portugal - USA ACGIH | ACGIH TWA (mg/m ³) | 5 mg/m ³ Upper Respiratory Tract irritation. ANS impairment. USA. ACGIH Threshold Limit Values (TLV) |
| USA OSHA | OSHA PEL (STEL) (mg/m ³) | 5 mg/m ³ California permissible exposure limits for chemical contaminants (Title 8, Article 107) |

8.2. Exposure controls

Appropriate engineering controls : Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment : Gloves. Protective clothing. Protective goggles. Self-contained breathing apparatus.



Materials for protective clothing : Wear suitable protective clothing and gloves.

Hand protection : Wear suitable protective clothing and gloves.

Eye protection : Wear safety glasses with side shields (or goggles) and a face shield.

Skin and body protection : Choose body protection according to the amount and concentration of the dangerous substance at the work place.

Respiratory protection : When appropriate, use NIOSH/CEN approved respirator.

Environmental exposure controls : Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

| | |
|---|---|
| Physical state | : Solid |
| Appearance | : Crystalline solid. |
| Molecular mass | : 150.17 g/mol (Labeled) |
| Color | : white. |
| Odor | : No data available |
| Odor threshold | : No data available |
| pH | : 2.7 at 23 g/l at 25 °C (77 °F) |
| Relative evaporation rate (butyl acetate=1) | : No data available |
| Melting point | : 151 - 154 °C (304 - 309 °F) |
| Freezing point | : No data available |
| Boiling point | : 265 °C (509 °F) at 133 hPa (100 mmHg) - lit. |
| Flash point | : 196 °C (385 °F) - closed cup |
| Self ignition temperature | : > 400 °C (> 752 °F) |
| Decomposition temperature | : No data available |
| Flammability (solid, gas) | : May form combustible dust concentrations in air. |
| Vapor pressure | : 1 hPa (1 mmHg) at 159.5 °C (319.1 °F); 0.097 hPa (0.073 mmHg) at 18.5 °C (65.3 °F) |
| Relative vapor density at 20 °C | : No data available |
| Relative density | : 1.46 g/cm ³ at 20 °C (68 °F) |
| Solubility | : Soluble in methanol. Slightly soluble in Benzene. Water: 23 g/l at 25 °C (77 °F) - soluble Ethanol: soluble Acetone: soluble |
| Log Pow | : 0.093 at 25 °C (77 °F) |
| Log Kow | : No data available |
| Viscosity, kinematic | : No data available |
| Viscosity, dynamic | : No data available |
| Explosive properties | : No data available |
| Oxidizing properties | : No data available |
| Explosive limits | : No data available |

9.2. Other information

No additional information available

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SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

Stable if stored under recommended conditions.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

No additional information available

10.5. Incompatible materials

Strong oxidizing agents.

10.6. Hazardous decomposition products

carbon oxides.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

| ADIPIC ACID (3,3,4,4-D4, 98%) (121311-78-2) | |
|---|--|
| LD50 oral rat | 5560 mg/kg male and female (OECD Test Guideline 401) |
| LD50 dermal rabbit | 7940 mg/kg male and female |
| LC50 inhalation rat (mg/l) | > 7.7 mg/l male and female - 4 h (OECD Test Guideline 403) |
| ATE (oral) | 4500.000 mg/kg body weight |

Skin corrosion/irritation : Not classified

No data available
pH: 2.7 at 23 g/l at 25 °C (77 °F)

Serious eye damage/irritation : Causes serious eye irritation.

No data available
pH: 2.7 at 23 g/l at 25 °C (77 °F)

Respiratory or skin sensitization : Maximisation Test - Guinea pig Result: Does not cause skin sensitization.

No data available

Germ cell mutagenicity : Hamster - fibroblast Result: Negative. . Rat - male Result: negative

Carcinogenicity : Not classified

Reproductive toxicity : Not available.

Specific target organ toxicity (single exposure) : Not classified

No data available

Specific target organ toxicity (repeated exposure) : Not classified

No data available

Aspiration hazard : Not classified

Potential Adverse human health effects and symptoms : To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Symptoms/injuries after inhalation : May be harmful if inhaled. Causes respiratory tract irritation.

Symptoms/injuries after skin contact : May be harmful if absorbed through skin. May cause skin irritation.

Symptoms/injuries after eye contact : Causes eye irritation.

Symptoms/injuries after ingestion : May be harmful if swallowed.

SECTION 12: Ecological information

12.1. Toxicity

| ADIPIC ACID (3,3,4,4-D4, 98%) (121311-78-2) | |
|---|---|
| LC50 fish 1 | >= 1000 mg/l static test LC50 - Brachydanio rerio (zebrafish) - 96 h |
| EC50 Daphnia 1 | 46 mg/l Immobilization LC50 - Daphnia magna (Water flea) - 48 h (OECD Test Guideline 202) |
| EC50 other aquatic organisms 1 | 7910 mg/l Respiration inhibition EC50 - Sludge Treatment - 3 h (OECD Test Guideline 209) |
| ErC50 (algae) | 59 mg/l static test EC50 - Pseudokirchneriella subcapitata (algae) - 72 h (OECD Test Guideline 201) |

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12.2. Persistence and degradability

| ADIPIC ACID (3,3,4,4-D4, 98%) (121311-78-2) | |
|---|---|
| Persistence and degradability | Aerobic - Exposure time 30 d. |
| Biodegradation | 83 % Readily biodegradable (OECD Test Guideline 301D) |

12.3. Bioaccumulative potential

| ADIPIC ACID (3,3,4,4-D4, 98%) (121311-78-2) | |
|---|--------------------------------------|
| BCF fish 1 | 80 ug/l - Lepomis macrochirus - 28 d |
| Bioconcentration factor (BCF REACH) | 1.8 |
| Log Pow | 0.093 at 25 °C (77 °F) |
| Bioaccumulative potential | Not available. |

12.4. Mobility in soil

| ADIPIC ACID (3,3,4,4-D4, 98%) (121311-78-2) | |
|---|----------------|
| Ecology - soil | Not available. |

12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Other adverse effects

Other adverse effects : An environmental hazard cannot be excluded in the event of an unprofessional handling or disposal. Harmful to aquatic life.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Regional legislation (waste) : Waste materials should be disposed of under conditions which meet Federal, State, and Local environmental control regulations.

Waste disposal recommendations : Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Ecology - waste materials : Dispose of as unused product.

SECTION 14: Transport information

In accordance with ADR / RID / ADNR / IMDG / ICAO / IATA

14.1. UN number

UN-No.(DOT) : 3077
DOT NA no. UN3077

14.2. UN proper shipping name

DOT Proper Shipping Name : Environmentally hazardous substances, solid, n.o.s.
(Adipic acid)

Department of Transportation (DOT) Hazard Classes : 9 - Class 9 - Miscellaneous hazardous material 49 CFR 173.140

Hazard labels (DOT) : 9 - Class 9 (Miscellaneous dangerous materials)



DOT Symbols : G - Identifies PSN requiring a technical name
Packing group (DOT) : III - Minor Danger

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- DOT Special Provisions (49 CFR 172.102) : 8 - A hazardous substance that is not a hazardous waste may be shipped under the shipping description "Other regulated substances, liquid or solid, n.o.s.", as appropriate. In addition, for solid materials, special provision B54 applies.
- 146 - This description may be used for a material that poses a hazard to the environment but does not meet the definition for a hazardous waste or a hazardous substance, as defined in 171.8 of this subchapter, or any hazard class as defined in Part 173 of this subchapter, if it is designated as environmentally hazardous by the Competent Authority of the country of origin, transit or destination.
- 335 - Mixtures of solids that are not subject to this subchapter and environmentally hazardous liquids or solids may be classified as "Environmentally hazardous substances, solid, n.o.s." UN3077 and may be transported under this entry, provided there is no free liquid visible at the time the material is loaded or at the time the packaging or transport unit is closed. Each transport unit must be leak-proof when used as bulk packaging.
- A112 - Notwithstanding the quantity limits shown in Column (9A) and (9B) for this entry, the following IBCs are authorized for transportation aboard passenger and cargo-only aircraft. Each IBC may not exceed a maximum net quantity of 1,000 kg:
- a. Metal: 11A, 11B, 11N, 21A, 21B and 21N
 - b. Rigid plastics: 11H1, 11H2, 21H1 and 21H2
 - c. Composite with plastic inner receptacle: 11HZ1, 11HZ2, 21HZ1 and 21HZ2
 - d. Fiberboard: 11G
 - e. Wooden: 11C, 11D and 11F (with inner liners)
 - f. Flexible: 13H2, 13H3, 13H4, 13H5, 13L2, 13L3, 13L4, 13M1 and 13M2 (flexible IBCs must be sift-proof and water resistant or must be fitted with a sift-proof and water resistant liner).
- B54 - Open-top, sift-proof rail cars are also authorized.
- IB8 - Authorized IBCs: Metal (11A, 11B, 11N, 21A, 21B, 21N, 31A, 31B and 31N); Rigid plastics (11H1, 11H2, 21H1, 21H2, 31H1 and 31H2); Composite (11HZ1, 11HZ2, 21HZ1, 21HZ2, 31HZ1 and 31HZ2); Fiberboard (11G); Wooden (11C, 11D and 11F); Flexible (13H1, 13H2, 13H3, 13H4, 13H5, 13L1, 13L2, 13L3, 13L4, 13M1 or 13M2).
- IP3 - Flexible IBCs must be sift-proof and water-resistant or must be fitted with a sift-proof and water-resistant liner.
- N20 - A 5M1 multi-wall paper bag is authorized if transported in a closed transport vehicle.
- T1 - 1.5 178.274(d)(2) Normal..... 178.275(d)(2)
- TP33 - The portable tank instruction assigned for this substance applies for granular and powdered solids and for solids which are filled and discharged at temperatures above their melting point which are cooled and transported as a solid mass. Solid substances transported or offered for transport above their melting point are authorized for transportation in portable tanks conforming to the provisions of portable tank instruction T4 for solid substances of packing group III or T7 for solid substances of packing group II, unless a tank with more stringent requirements for minimum shell thickness, maximum allowable working pressure, pressure-relief devices or bottom outlets are assigned in which case the more stringent tank instruction and special provisions shall apply. Filling limits must be in accordance with portable tank special provision TP3. Solids meeting the definition of an elevated temperature material must be transported in accordance with the applicable requirements of this subchapter.
- DOT Packaging Exceptions (49 CFR 173.xxx) : 155
- DOT Packaging Non Bulk (49 CFR 173.xxx) : 213
- DOT Packaging Bulk (49 CFR 173.xxx) : 240

14.3. Additional information

- Other information : No supplementary information available.
- Special transport precautions : Not dangerous goods.

Overland transport

- Packing group (ADR) : III
- Class (ADR) : 9 - Miscellaneous dangerous substances and articles
- Hazard identification number (Kemler No.) : 90
- Classification code (ADR) : M7
- Danger labels (ADR) : 9 - Miscellaneous dangerous compounds



- Orange plates : 

- Tunnel restriction code : E
- Limited quantities (ADR) : 5kg

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EAC : 2Z
Excepted quantities (ADR) : E1

Transport by sea

DOT Vessel Stowage Location : A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.
MFAG-No : 171

Air transport

DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) : No limit
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : No limit
Civil Aeronautics Law : Miscellaneous dangerous substances & articles

14.4. Environmental hazards

Other information : No supplementary information available.

14.5. Special precautions for user

Special transport precautions : Not dangerous goods.

14.6. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

SECTION 15: Regulatory information

15.1. US Federal regulations

ADIPIC ACID (3,3,4,4-D4, 98%) (121311-78-2)

| | |
|-------------------------------------|---------------------------------|
| SARA Section 311/312 Hazard Classes | Immediate (acute) health hazard |
|-------------------------------------|---------------------------------|

15.2. International regulations

CANADA

No additional information available

15.2.1. National regulations

No additional information available

15.3. US State regulations

ADIPIC ACID (3,3,4,4-D4, 98%)(121311-78-2)

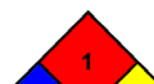
| | |
|----------------------------|---|
| State or local regulations | U.S. - Massachusetts - Right To Know List U.S. - Pennsylvania - RTK (Right to Know) List U.S. - New Jersey - Right to Know Hazardous Substance List This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm. |
|----------------------------|---|

SECTION 16: Other information

Full text of R-, H- and EUH-phrases::

| | |
|--------------|--|
| Eye Irrit. 2 | Serious eye damage/eye irritation Category 2 |
| H319 | Causes serious eye irritation |
| R36 | Irritating to eyes |
| R52 | Harmful to aquatic organisms |
| Xi | Irritant |

NFPA health hazard : 2 - Intense or continued exposure could cause temporary incapacitation or possible residual injury unless prompt medical attention is given.



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NFPA fire hazard : 1 - Must be preheated before ignition can occur.
NFPA reactivity : 0 - Normally stable, even under fire exposure conditions,
and are not reactive with water.

HMIS III Rating

Health : 2 Moderate Hazard - Temporary or minor injury may occur
Flammability : 1 Slight Hazard
Physical : 0 Minimal Hazard

CIL Multi-Solvent Mixture SDS

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product